II International Conference on Particle-based Methods - Fundamentals and Applications
PARTICLES 2011
E. Oñate and D.R.J. Owen (Eds)

PARTICLE HYDRODYNAMICS: FROM MOLECULAR TO COLLOIDAL FLUIDS

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Key words: particle hydrodynamics, Eulerian-Lagrangian method, fluctuating hydrodynamics

Abstract. A method for particle hydrodynamics based on an hybrid Eulerian-Lagrangian approach is presented. Particles are solved in the continuum space while the fluid is solved in an Eulerian mesh, and described by finite volume fluctuating hydrodynamics. This set-up is particulary suited for micron-size devices where the Reynolds number is small but thermal fluctuations are important. The fluid-particle coupling force is obtained by imposing zero relative (particle-fluid) velocity at discrete points representing the particle sites. In this work particles are described by an only site which neglect rotation. The momentum exchanged between fluid and particle is transfered instantaneously and this brings about several benefits such as a correct treatment of inertia and proper particle velocity fluctuations uniquely driven by the fluid thermal forces. The present scheme is designed for incompressible and compressible fluids at low Mach number. This is theoretically shown by analyzing the consistency between the Eulerian and Lagrangian momentum balance.A series of tests up to moderate Reynolds number and acoustic forces under ultrasound waves are also presented.

1 INTRODUCTION

The emergence of complex phenomena is common aspect in particle hydrodynamics. An example is the collective motion of a swarm of particles immersed in a fluid, interacting among them with short-ranged potentials and also along larger distances, via the hydrodynamic field [1]. Numerical simulations constitute a powerful tool to isolate and dissect the effect of each force or detail, in ways that cannot be experimentally reproduced. Computational studies of this sort certainly requires some type of simplification or *coarse-graining* procedure. A hierarchical list of simplifications might be envisaged, starting from the elimination of the molecular degrees of freedom of the solvent and concluding by the

gradual simplification of the solute particle structure up to a single "point" moving in space (the so called *point particle* approximation [2]). In performing this reductionist approach one needs to consider several important constraints: consistent momentum (and energy) conservation and hydrodynamic fluctuations if dealing with micron or submicron size systems (in such case convection does not make a significant contribution).

There are three general schemes to face the general problem of particle hydrodynamics: fully Eulerian , fully Lagrangian methods and Eulerian-Lagrangian hybrids. Treating both particle and solvent within an Eulerian grid demands solving the delicate technical problem of adapting the grid (remeshing) around the moving particle. A more natural approach might be to use fully Lagrangian schemes, based for instance in Smooth Particle Hydrodynamics. These have been evolving in complexity and have been recently generalized to non-Newtonian fluids [5]. Here we focus on the third approach whereby the fluid is solved in the (probably faster) fixed Eulerian grid, while particles move in the continuum space. Ideas from these three approaches start to spread (SPH with remeshing steps are now used [6] and maybe, SPH interpolation kernels could adapted to Eulerian-Lagrangian methods)

The kernel function is key to properly solve the particle hydrodynamics. It is in charge of the two essential communications: how to spread local (surface or point) forces over the fluid and how to interpolate fluid variables at desired (particle) point. We adhere to the interpolation kernels derived for the Immersed Boundary method [7] and show they are flexible enough to ensure consistency in the force and velocity coupling. Another key issue is the ansatz used for the particle-fluid force. This determines the physics the method will be able to tackle. In particular, in the IB method the particle (or surface point) velocity $\dot{\mathbf{R}}$ simply follows the local fluid interpolated value $\mathbf{u}$, meaning that inertial forces are absent. The exchanged forces arise from the distortion of the particle-particle potential energy as in fact, an isolated particle would have trivial $\dot{\mathbf{R}} = \mathbf{u}$ dynamics. If one is interested in tracing non-bonded particles another strategy is thus required. A common one is to construct a force inspired on the zero Reynolds form of the Stokes drag, $\mathbf{F} = \xi(\dot{\mathbf{R}} - \mathbf{u})$, providing a fluid-particle force and non-trivial dynamics $\ddot{\mathbf{R}} = \mathbf{F}/M$ for particle with mass M. If fluctuations are important, the damping force used for the particle-fluid coupling makes necessary the usage of a noise term in the particle equation to ensure the correct equilibrium kinetic temperature of the particles [2]. The Stokes coupling introduces a friction time M/ξ which limits the fastest process one can resolve. A number of interesting applications of polymeric and colloidal suspensions in micro-flow devices however require relative large flow change rates and velocity gradients of the same order of the particle radius for which the Stokes friction limit neither valid. Applications involving ultrasound are now flourishing, such as manipulation or treatment of micron size particles using ultrasound, with important technological applications [3]. In this report we present an extension to the above ideas where particle and fluid motion are coupled in the strongly overdamped limit, i.e. the fluid-particle transfer of momentum is instantaneous. This method, called Direct Forcing, obtains the fluid-particle force upon imposition of

the no-slip fluid velocity at a *single* particle site. This work extends previous Direct Forcing approaches [4] to point-wise particles, giving a precise meaning of the particle effective volume, and comparing for consistency the Eulerian and Lagrangian versions of momentum conservation.

2 Equations of motion

Consider an spherical particle of mass M_p immersed in a fluid. The particle center is located at $\mathbf{R}_p(t)$, it has surface S_p and volume $\mathcal{V}_p$. The force on the particle due to the fluid is given by the sum of the fluid pressure over the particle surface, $-\oint_S \mathcal{P}\cdot\mathbf{n}d\mathbf{r}^2$. Using the divergence theorem, the particle equation of motion results in

$$M_p\frac{d\mathbf{V}_p}{dt} = -\int_{\mathcal{V}_p}\nabla\cdot\mathcal{P}\mathrm{d}\mathbf{r}^3 + \mathbf{F}_{\mathrm{ext}} \tag{1}$$

where $\mathbf{V}_p = \dot{\mathbf{R}}_p$. An extra force $\mathbf{F_{ext}}$ has been added to represent any external field and/or interaction with other particles. In what follows we focus on particle translation and ignore particle rotation. Extensions to include rotational degrees of freedom are underway. We also consider a Newtonian fluid in isothermal environment for which the conservation equations of mass density $\rho(\mathbf{r},t)$ and momentum density $\mathbf{g}(\mathbf{r},t) = \rho\mathbf{u}$ are

$$\frac{\partial\rho}{\partial t} = -\nabla\cdot\mathbf{g} \tag{2}$$

$$\frac{\partial\mathbf{g}}{\partial t} = -\nabla\cdot\mathbf{\Pi} + \mathbf{f}. \tag{3}$$

Where the stress tensor $\mathbf{\Pi} = \mathbf{gu}+\mathcal{P}$ includes the convective term and $\mathcal{P} = \pi\mathbf{1}+\eta[\nabla\mathbf{u}]^{\mathtt{sym}}+\tilde{\mathcal{P}}$ contains an scalar pressure π a diffusive term (the symmetrized tensor is indicated as $A^{\mathtt{sym}} = (A+A^T)/2$) and a fluctuating component of thermal origin. Fluctuating hydrodynamics described by Eqs. (2) and (3) were solved using the finite volume method in a regular mesh. Details can be found in Ref. [8]. In general, the density force $\mathbf{f}$ arises from the fluid-particle interaction, ensures fulfillment of the velocity boundary condition at the particle surface and the exclusion of fluid from the particle inside. These boundary equations require resolving the particle surface (using a set of points at the surface) [4]. By contrast the intention here is to simplify the particle description up to being described by a single point at its center and an effective volume $\mathcal{V}_p$. The boundary condition for the fluid velocity is thus,

$$\mathbf{u}(\mathbf{R}_p) = \mathbf{V}_p \tag{4}$$

where $\mathbf{V}_p = \dot{\mathbf{R}}_p$ is the particle velocity. Finally in this point-wise approximation, the fluid leaks into or entrain the particle. In other words, no boundary condition is imposed inside or at the particle domain.

2.1 Force balance and momentum conservation

Instead of directly dealing with the integral of the divergence of the pressure tensor to solve the particle dynamics described by Eq. (1), it is much easier to reformulate the problem in terms of global momentum conservation. More generally, consider that the fluid contains a number of particles $p = \{1, ..., M\}$ located at $\{\mathbf{R}_p\}$. One can integrate Eq. (3) over the whole domain to obtain the rate of change of total fluid momentum

$$\frac{d}{dt}\int \mathbf{g}\,\mathrm{d}\mathbf{r}^3 = \int \nabla\cdot\mathcal{P}\,\mathrm{d}\mathbf{r}^3 + \int \mathbf{f}\,\mathrm{d}\mathbf{r}^3 \tag{5}$$

We shall assume that the fluid-particle interaction is local and short ranged, with a cutoff radius of microscopic size. This means that the force $\mathbf{f}$ only differs from zero around a shell infinitely close to each particle surface. The volume of this shell around one particle p is denoted $\mathcal{V}_p$. Under this assumption

$$\int \mathbf{f}\mathrm{d}\mathbf{r}^3 = \int_{\cup\mathcal{V}_p} \mathbf{f}\mathrm{d}\mathbf{r}^3 = \sum_p \int_{\mathcal{V}_p} \mathbf{f}\mathrm{d}\mathbf{r}^{\mathbf{3}}. \tag{6}$$

For the last equality we assume *non-overlapping* particle volumes, which follows from the fact that particles cannot interpenetrate. The total force due to particle p is denoted as, $\mathbf{F}_p = \int_{\mathcal{V}_p} \mathbf{f}\mathrm{d}\mathbf{r}^{\mathbf{3}}$ so that the total force on the fluid due to the particles is

$$\sum_p \mathbf{F}_p = \int \mathbf{f}\mathrm{d}\mathbf{r}^{\mathbf{3}} \tag{7}$$

To derive a dynamic equation for the particle p we integrate Eq. (3) over the particle volume $\mathcal{V}_p$ and insert Eq. (1) to get,

$$M_p\frac{d\mathbf{V}_p}{dt} = \frac{d}{dt}\int_{\mathcal{V}_p} \mathbf{g}\,\mathrm{d}\mathbf{r}^3 - \int_{\mathcal{V}_p} \mathbf{f}\,\mathrm{d}\mathbf{r}^3 + \mathbf{F}_{\text{ext}} \tag{8}$$

For an incompressible fluid of density ρ, momentum conservation *inside* the particle ensures that [4], $\frac{d}{dt}\int_{\mathcal{V}} \mathbf{g}\,\mathrm{d}\mathbf{r}^3 = \rho\,\frac{d}{dt}[\int_{\mathcal{V}} \mathbf{u}\,\mathrm{d}\mathbf{r}^3] = m_p\frac{d\mathbf{V}_p}{dt}$ where the $m_p = \rho\mathcal{V}$ is the fluid mass the particle evacuates. The Archimedes force is thus recovered,

$$\Delta M_p\frac{d\mathbf{V}_p}{dt} = -\mathbf{F}_p + \mathbf{F}_{\text{ext}} \tag{9}$$

The mass excess $\Delta M_p = M_p - m_p$ is indeed constant for an incompressible fluid, so fixing ΔM_p means defining the particle mass $M_p = \Delta M_p + \rho\mathcal{V}$. In Eq. (9) we have defined $\mathbf{F}_p$ as the total force exchanged between the fluid and the particle p. Note that Eq. (9) ensures that the total momentum of the system is conserved.

2.2 The particle-fluid force

As stated, the central idea of the direct forcing scheme is to obtain the fluid-particle interaction force $\mathbf{F}_p$ from the imposition of the no-slip boundary condition at the particle site $\mathbf{R}_p$. As particles do not overlap, the total force exchanged between the fluid and the whole set of particles is just the sum of each individual particle contribution, as stated in Eq. (7). Let us then derive the force due to one particle p. The fluid momentum variation due to such force $\mathbf{F}_p$ over time interval Δt is given by the integral of Eq. (3) over $\mathcal{V}_p$ and Δt. Let us now focus on incompressible fluids $\mathbf{g}(\mathbf{r}) = \rho\mathbf{u}(\mathbf{r})$ to get,

$$\rho\langle\mathbf{u}\rangle_p(t+\Delta t) = \rho\tilde{\mathbf{u}}_p + \frac{1}{\mathcal{V}_p}\int_t^{t+\Delta t}\mathbf{F}_p(t')\mathrm{d}t'. \tag{10}$$

The amount of any (extensive) quantity inside the particle domain is noted as $\langle\phi\rangle_p\,\mathcal{V}_p \equiv \int_{\mathcal{V}_p}\phi\mathrm{d}\mathbf{r}^3$ and defines the volume averaged quantities (for instance, $\langle\mathbf{g}\rangle_p = \rho\langle\mathbf{u}\rangle_p$ is the averaged momentum density inside $\mathcal{V}_p$). Equation (10) also introduces,

$$\rho\tilde{\mathbf{u}}_p = \rho\langle\mathbf{u}\rangle_p(t) - \int_t^{t+\Delta t}\langle\nabla\cdot\boldsymbol{\Pi}\rangle_p(t')\mathrm{d}t', \tag{11}$$

which is the average momentum density that fluid would have had in the particle domain if no particle constraint would have been imposed during the time interval. In this sense $\tilde{\mathbf{u}}$ is called *unperturbed* fluid velocity. Imposing the "stick" constraint $\langle\mathbf{u}\rangle_p = \mathbf{V}_p$ in Eq. (10) yields the following integral restriction to the force,

$$\int_t^{t+\Delta t}\mathbf{F}_p(t')\mathrm{d}t' = \rho\mathcal{V}_p\left[\mathbf{V}_p(t+\Delta t) - \tilde{\mathbf{u}}_p\right]. \tag{12}$$

Equation (12) is the change of fluid momentum over Δt due to the presence of the particle p. Generalization to many *non-overlapping* particles is straightforward, as stated in Eq. (7).

3 Implementation

Equations (5)-(12) constitute the core of the particle hydrodynamics problem we intend to solve. To that end, the next ingredient to add is the so called "point-particle" approximation, which formally consists on approximating the volume average $\langle\phi\rangle_p$ by an interpolated value ϕ_p at some location (for spherical particles in incompressible fluid, the particle center) in the particle domain $\mathcal{V}_p$. For this task we use the kernel function developed for the Immersed Boundary Method (IBM)[7]. On the other hand, in this work we use a first order explicit scheme (forward Euler) to integrate the equations in time. Both issues are now discussed.

3.1 Interpolation and Spreading

The Eulerian-Lagrangian mixed approach moves the particle in the continuum (Lagrangian) space while the fluid is solved in a fixed Eulerian mesh. Any Eulerian fluid solver (based either on finite differences, finite volumes or even the Lattice-Boltzmann method) can be used. The set of $i = \{1, ..., N\}$ fluid nodes are located at $\{\mathbf{r}_i\}$ fluid nodes. On the other hand there are $p = \{1, ..., M\}$ particles at sites $\{\mathbf{R}_p\}$. Communication between Eulerian and Lagrangian dynamics require two central operations. First, the evaluation of the fluid-particle force in Eq. (12) requires the *interpolation* of the unperturbed fluid velocity at the particle site and, second, this force has to be *spread* to the surrounding fluid nodes (so that Eq. (10) is fulfilled at each particle site). These two operations are respectively performed by the operators $\delta^I(\mathbf{s})$ and $\delta^S(\mathbf{s})$ which can be generally defined as convolution integrals in the continuum space [7]. As we are focusing on discrete (point-wise) particles it is more natural to express these operations in its discrete form,

$$\phi_p^I = \sum_i \delta_{ip}^I \phi_i \text{ and } \phi_i^S = \sum_p \delta_{ip}^S \phi_p \tag{13}$$

where $\phi_i = \phi(\mathbf{r}_i)$ and $\phi_p = \phi(\mathbf{R}_p)$. The spreading and interpolators are constructed like $\delta^I(\mathbf{r}) = \delta_h(x)\delta_h(y)\delta_h(z)$ where $\delta_h(s)$ is the three point kernel discussed in Ref. [7]. In any case $\delta_{ip}^I = \delta^I(|\mathbf{r}_i - \mathbf{R}_p|)$ (similarly for δ^S). The following properties hold:

$$\sum_i h^3 \delta_{ip}^I = h^3 \tag{14}$$

$$\sum_i h^3 \delta_{ip}^S = \mathcal{V}_p \tag{15}$$

It is also particularly important that the composition of spreading and interpolation yields the identity. Starting from any Lagrangian variable, ϕ_p: spread gives $\phi_i^S = \sum_p \phi_p \delta_{ip}^S$ and interpolation $\phi_p^{SI} = \sum_q [\sum_i \delta_{ip}^I \delta_{iq}^S] \phi_q$. Therefore $\phi_p^{SI} = \phi_p$ if

$$\sum_i \delta_{ip}^I \delta_{iq}^S = \delta_{pq}^{\mathrm{kr}} \tag{16}$$

Where $\delta_{pq}^{\mathrm{kr}}$ is the Kronecker delta. As discussed by Peskin [7], the kernels satisfy a softer property, namely $\sum_i \delta_{ip}^I \delta_{ip}^S = 1$ However, as they only differ from zero within a finite width ($2h$ in our implementation), in practice, Eq. (16) strictly holds if particles cannot not overlap. This can be ensured either by lubrication or (steric) repulsive interparticle potentials.

3.2 Integration

The particle and fluid equations of motion will be integrated using a time step Δt. The discrete set of times is noted as $t_n = n\Delta t$. We now follow the sequence of steps of the

algorithm hereby derived although for now, we keep time integrals by introducing this notation,

$$\overline{\phi} \equiv \frac{1}{\Delta t}\int_{t_n}^{t_{n+1}} \phi(t)\mathrm{d}t \tag{17}$$

- Following the same line leading to Eqs. (10) and (11), the first step of the algorithm derives the unperturbed Eulerian velocity,

$$\rho\tilde{\mathbf{u}}_i = \rho\mathbf{u}_i^n - \overline{[\nabla\cdot\mathbf{\Pi}]}_i\Delta t \tag{18}$$

  where $\mathbf{u}_i^n = \mathbf{u}(\mathbf{r}_i, t_n)$, etc.

- The Eulerian unperturbed velocity is interpolated at the Lagrangian sites $p = \{1, ..., M\}$. It is important to note that the interpolator and spreading operators depend on time via the particle position. We shall indicate this dependence in the particle subscript, e.g. $\delta^I_{ip^n} = \delta^I(|\mathbf{r}_i - \mathbf{R}_p(t_n)|)$. The updated particle positions $\mathbf{R}_p^{n+1} = \mathbf{R}_p^n + \overline{\mathbf{V}}_p\Delta t$ are used to evaluate the interpolated unperturbed velocity

$$\tilde{\mathbf{u}}_p = \sum_i \delta^I_{ip^{n+1}}\tilde{\mathbf{u}}_i \tag{19}$$

- The updated particle velocity is obtained upon integration of Eq. (9) where the fluid-particle force in turn depends on the particle velocity. However Eq. (12) introduces the integrated effect of this force instantaneously at the end of the integration step (time t_{n+1}). This fact and the assumption of non-overlapping kernels simplify the (otherwise transcendental) equation (9) and (12) to a linear system for $\mathbf{V}_p$ and $\mathbf{F}_p$ which can be solved in a single step (i.e. without costly iterations). The updated particle velocity results,

$$\mathbf{V}_p^{n+1} = \mathbf{V}_p^n + \frac{m_p}{\Delta M_p + m_p}\left(\tilde{\mathbf{u}}_p - \mathbf{V}_p^n\right) + \frac{\overline{\mathbf{F}_{\text{ext}}}\Delta t}{\Delta M_p + m_p}. \tag{20}$$

  The fluid mass within the particle domain is denoted as $m_p = \mathcal{V}_p\sum_i \rho_i\delta^I_{ip}$; for an incompressible fluid $m_p = \rho\mathcal{V}_p$.

- The particle-fluid force is now spread to the Eulerian nodes. As before, the volume integral over one fluid cell of volume h^3 is $\int_{h^3}\mathbf{f}(\mathbf{r})\mathrm{d}r^3 \simeq \mathbf{f}_i h^3$. So from Eq. (7) the net gain in fluid momentum due to the particle presence is,

$$\sum_i \int_{t_n}^{t_{n+1}} \mathbf{f}_i\mathrm{d}t'\, h^3 = \sum_p \int_{t_n}^{t_{n+1}} \mathbf{F}_p\mathrm{d}t' \tag{21}$$

  Equation (21) provides consistency between the interpolated Lagrangian forces and the Eulerian momentum gain (the consistency between spread Eulerian forces and

the Lagrangian momentum gain is discussed in next Section). The spreading operation should therefore ensure fulfillment of Eq. (21). To that end, the net momentum gain in the fluid due to the immersed particles is decomposed in individual particle contributions (i.e. $\mathbf{f}_i = \sum_p \mathbf{f}_{ip}$). Following Eqs. (7) and (12) leads to,

$$\int_{t_n}^{t_{n+1}} \mathbf{f}_{ip}(t')\mathrm{d}t' = \rho \left[\mathbf{V}_p^{n+1} - \tilde{\mathbf{u}}_p\right] \delta^S_{ip^{n+1}} \tag{22}$$

which satisfies Eq. (21) provided that the spreading property (15) holds. One can finally add the particle's spread momentum given by Eq. (22) to the unperturbed fluid momentum of each node "i" to get

$$\mathbf{u}_i^{n+1} = \tilde{\mathbf{u}}_i + \sum_p \left(\mathbf{V}_p^{n+1} - \tilde{\mathbf{u}}_p\right) \delta^S_{ip^{n+1}} \tag{23}$$

An important test of the scheme is to ensure that the fluid velocity at Lagrangian site p obtained by interpolation of Eq. (23) yields the desired particle value. Multiplying Eq. (23) by $\delta^I_{ip^{n+1}}$ and summing over i leads to, $\mathbf{u}_p = \tilde{\mathbf{u}}_p + \sum_q \left(\mathbf{V}_q - \tilde{\mathbf{u}}_q\right) \sum_i \delta^I_{ip}\delta^S_{iq}$. Thus $\mathbf{u}_p = \mathbf{V}_p$ is satisfied provided that the already highlighted Eq. (16) holds.

4 Consistency: compressible fluids at Low Mach number

In this section we analyze the consistency between Eulerian and Lagrangian forces-momentum conversion. To illustrate this point we consider a more general case: particles immersed in a compressible fluid. As an outcome we prove that a trivial modification of the present scheme [whereby the uniform density ρ is substituted by node values ρ_i, in Eqs. (18) and (22)] is perfectly valid under low Mach number. This fact was confirmed in simulations.

The consistency one would like to achieve in the discretized scheme builds up from the local character of the fluid-particle force field $\mathbf{f}$ reflected in Eq. (6). This relation implies that the gain in fluid momentum due the particles presence can be equally obtained either by integrating over the whole fluid domain or by integration over the set of non-overlapping particle volumes $\cup\mathcal{V}_p$. For consistency, these two integrals should be equal in the numerical scheme: while the first integral (over the whole volume) is carried out with Eulerian variables, the second one (over particle volumes) corresponds to Lagrangian counterparts. To begin with, the fluid momentum introduced at one Eulerian node "i" by the particles over Δt is,

$$h^3 \left(\Delta \mathbf{g}_i + \overline{[\nabla \cdot \mathbf{\Pi}]}_i \Delta t\right) = \sum_p h^3 \overline{\mathbf{f}_{ip}} \Delta t \tag{24}$$

The total momentum gain is obtained by integrating over the whole domain. Its discretized Eulerian version is $\Delta \mathbf{W}_\mathrm{E} = h^3 \sum_i \left(\Delta \mathbf{g}_i + \overline{\nabla \cdot \mathbf{\Pi}}]_i \Delta t\right)$ where,

$$\Delta \mathbf{W}_\mathrm{E} = \sum_i \sum_p h^3 \overline{\mathbf{f}_{ip}} \Delta t = \sum_p \overline{\mathbf{F}}_p \Delta t \tag{25}$$

The second equality is just Eq. (21) which, as stated, is guaranteed by the spreading property (15).

Before performing the force integral over the set of particle volumes, let us trivially generalize the spread force in Eq. (22) to a compressible density field, $\{\rho_i\}$,

$$\overline{\mathbf{f}_{ip}}\Delta t = \rho_i \left[\mathbf{V}_p - \tilde{\mathbf{u}}_p\right] \delta^S_{ip}. \tag{26}$$

Now, as stated above, in the point particle approximation the integral over the particle volume $\int_{\mathcal{V}_p} \phi(\mathbf{r})\mathrm{d}r^3$ is given by $\phi_p \mathcal{V}_p$ where ϕ_p is a (interpolated) *Lagrangian* variable. To obtain the Lagrangian expression for the change of fluid momentum due to the particle p we interpolate of Eq. (24) at $\mathbf{R}_p(t+\Delta t)$, add and extract $\mathbf{g}^n_p$ to get,

$$\Delta \mathbf{g}_p + \left[\overline{\nabla \cdot \mathbf{\Pi}}\right]_{p^{n+1}} \Delta t = \left(\mathbf{g}^n_{p^{n+1}} - \mathbf{g}^n_{p^n}\right) + \mathcal{V}_p^{-1}\overline{\mathbf{F}^*_p}\Delta t \tag{27}$$

Where we have introduced the notation $\mathbf{g}^n_{p^{n+1}} = \sum_i \mathbf{g}^n_i \delta^I_{ip^{n+1}}$ to express a Eulerian field at time t_n interpolated at the particle position $\mathbf{R}_p(t_n+\Delta t)$ in the updated time. Whenever both times coincides we simplify the notation, $\mathbf{g}^{n+1}_{p^{n+1}} = \mathbf{g}^{n+1}_p$ and indeed $\Delta \mathbf{g}_p = \mathbf{g}^{n+1}_p - \mathbf{g}^n_p$.

The modified particle force appearing in Eq. (27) arises from the force density chosen in Eq. (26), $\mathcal{V}_p^{-1}\overline{\mathbf{F}^*_p}\Delta t = \sum_i \overline{\mathbf{f}_{ip}}\delta^I_{ip^{n+1}}\Delta t$, resulting in

$$\overline{\mathbf{F}^*_p}\Delta t = \mathcal{V}_p \rho^*_p \left[\mathbf{V}^{n+1}_p - \tilde{\mathbf{u}}_p\right] \text{ with} \tag{28}$$

$$\rho^*_p = \sum_i \rho_i \delta^I_{ip}\delta^S_{ip} \tag{29}$$

Before dealing with this force, let us first analyze the new convective term appearing in Eq. (27). Introducing the Lagrangian spatial derivative $\nabla_{\mathbf{R}}\phi \cdot \mathrm{d}\mathbf{R} = \phi(\mathbf{R}+\mathrm{d}\mathbf{R}) - \phi(\mathbf{R})$ leads to,

$$\mathbf{g}^n_{p^{n+1}} - \mathbf{g}^n_{p^n} = \nabla_{\mathbf{R}}\, \mathbf{g}^n_p \cdot \overline{\mathbf{V}_p}\, \Delta t = \left(\nabla \cdot \left[\mathbf{g}^n_p \overline{\mathbf{V}_p}\right) - \overline{\mathbf{V}_p}\nabla_{\mathbf{R}} \cdot \mathbf{g}^n_p\right]\, \Delta t \tag{30}$$

For an incompressible fluid $\partial_t \rho_p = -\nabla \cdot \mathbf{g}_p = 0$ and the second term vanishes. In the compressible case it is not difficult to see that the last term of Eq. (30) simplifies out [1] Extracting the convective term from the stress tensor $\mathbf{\Pi} = \mathbf{g}\mathbf{u} + \mathcal{P}$ leads to

$$\Delta \mathbf{g}_p + \overline{\nabla_{\mathbf{R}} \cdot \mathcal{P}_{p^{n+1}}}\Delta t = \nabla_{\mathbf{R}} \cdot \left(\mathbf{g}^n_p \overline{\mathbf{V}_p} - \overline{[\mathbf{g}\mathbf{u}]}_{p^{n+1}}\right)\, \Delta t + \overline{\mathbf{F}^*_p}\mathcal{V}_p^{-1}\Delta t \tag{31}$$

where we have used that $[\nabla \cdot \phi]_p = \nabla_{\mathbf{R}} \cdot \phi_p$ [2] and also used that $\mathcal{P}$ is linear. Alternatively, by also adding and extracting $\left[\overline{\nabla \cdot \mathbf{\Pi}}\right]_{p^n} \Delta t$ to Eq. (27) leads to,

$$\Delta \mathbf{g}_p + \overline{\nabla_{\mathbf{R}} \cdot \mathcal{P}_{p^n}}\Delta t = \nabla_{\mathbf{R}} \cdot \left(\tilde{\mathbf{g}}_{p^n} \overline{\mathbf{V}_p} - \overline{[\mathbf{g}\mathbf{u}]}_{p^n}\right) + \overline{\mathbf{F}^*_p}\mathcal{V}_p^{-1}\Delta t \tag{32}$$

[1] To see this one can decompose $\phi_i = \phi_p + \delta\phi_i$ (so that $\delta\phi_p = 0$ by construction). Then in the LHS of Eq. (31) $\Delta \mathbf{g}_p = \mathbf{g}^{n+1}_p - \mathbf{g}^n_p = \mathbf{u}^n_p \Delta\rho_p + \rho^{n+1}_p \Delta \mathbf{u}_p + \Delta[\delta\rho\delta\mathbf{u}]_p$. For the explicit scheme we are using $\Delta\rho_p = -\nabla_{\mathbf{R}} \cdot \mathbf{g}^n_p\, \Delta t$ and $\bar{\mathbf{V}}_p = \mathbf{V}^n_p = \mathbf{u}^n_p$. Therefore the last term at RHS of Eq. (30) simplifies out, but still one is left with a momentum contribution due to the convection of density-velocity correlations inside the kernel.

[2] This comes from the fact that the interpolator only depends on distances $|\mathbf{r}-\mathbf{R}|$, so the interpolation of a shifted function is just $\sum_i \phi(x_i+dx)\delta^I(|x_i - X|) = \sum_i \phi(x_i+dx)\delta^I(|x_i+dx-(X+dx)|) = \phi^I(X+dx)$.

At this point it is instructive to consider $\mathbf{F}_p^* = 0$, i.e., no particle in the fluid. In this case Eq. (31) should ideally provide the Lagrangian motion of a fluid parcel determined by the material derivative $\rho D\mathbf{u}/Dt = -\nabla_{\mathbf{R}}\mathcal{P}$. One finds however that the convective terms in the right hand side (RHS) of Eq. (31) do not exactly cancel out for two reasons. The first is unavoidable and comes out from the finite width of the kernels used. In other words $[\mathbf{gu}]_p = \mathbf{g}_p\mathbf{u}_p + [\delta\mathbf{g}\delta\mathbf{u}]_p$ so (the divergence of) momentum-velocity correlations inside the kernel domain contribute in the "parcel" equation of motion. The second source of error comes from the different momentum field encountered by the particle before and after each jump in position, during its discrete time integration. For our explicit scheme $\overline{\phi}_p = \phi_p^n$ the RHS of Eq. (31) becomes [3] of order $\rho u^3\Delta t^2/h^2$ and it is smaller than the viscous term on the LHS ($\rho\nu u\Delta t/h^2$) if Re$=uh/\nu < 1/C$ where $C = u\Delta t/h$ is the Courant number $C < 1$.

Expressing the momentum balance in the form of Eq. (32) more clearly indicates that this term is the momentum convected by the particle in space and time (indeed it contains the memory of the particle induced forces).

In conclusion the scheme yields the following total momentum change from the Lagrangian variables,

$$\Delta\mathbf{W}_{\mathrm{L}} = \sum_p \overline{\mathbf{F}_p^*}\,\Delta t + O(\rho u^3\Delta t^2/h^2) \tag{33}$$

Equation (33) with (28) and (29), is the *Lagrangian* version of the *Eulerian* momentum balance in Eq. (25). Up to the O(Δt^2) difference, whenever $\mathbf{F}_p^* \neq \mathbf{F}_p$, some inconsistency is introduced in the Eulerian-Lagrangian force transformation. In the incompressible formulation $\rho_i = \rho$, Eq. (29) ensures consistency between the Eulerian and Lagrangian total momentum $\Delta\mathbf{W}_{\mathrm{E}} = \Delta\mathbf{W}_{\mathrm{L}}$ provided the celebrated condition (16) holds.

Any inconsistency in the Lagrangian momentum balance will affect the meaning of the particle "mass" because it can only be dynamically understood (force/acceleration). Fortunately, the property (16) tell us that $\delta^I_{ip}\delta^S_{ip}$ is also an interpolator which satisfies (14) so one should expect $\rho_p \simeq \rho_p^*$ and $\mathbf{F}_p^* \simeq \mathbf{F}_p$. One can always write, $\overline{\mathbf{F}_p^*} = \overline{\mathbf{F}_p} + (m_p^* - m_p)\boldsymbol{\alpha}_p$ with $\boldsymbol{\alpha}_p\Delta t = \mathbf{V}_p - \tilde{\mathbf{u}}$. The fluid mass "inside" the particle are $m_p = \rho_p\mathcal{V}_p$ and $m_p^* = \rho_p^*\mathcal{V}_p$. It can be shown that this force difference $\delta\mathbf{F} = (m_p^* - m_p)\boldsymbol{\alpha}_p$ satisfies $\delta F/F < \delta\rho^{\max}/\rho_p \sim \mathrm{Ma}^2$, where $\delta\rho^{\max}$ is the maximum density disturbance and Ma is the Mach number. In other words the scheme modified according to Eq. (26 is valid in the low Mach regime. Alternative implementation allowing arbitrary Mach and this will be presented elsewhere.

5 Results

We have performed a series of simulations to check the behavior of the present scheme. The first task consisted on measuring the hydrodynamic radius of the particle. As also happens in other Eulerian-Lagrangian solvers for point-wise particles (based on Stokes

[3] Ignoring correlations it results $\nabla_{\mathbf{R}}\cdot\left(\mathbf{g}_p\mathbf{u}_p - \mathbf{g}_{p^{n+1}}\mathbf{u}_{p^{n+1}}\right)\Delta t = \nabla_{\mathbf{R}}\cdot\left(\nabla_{\mathbf{R}}(\mathbf{g}_p\mathbf{u}_p)\cdot\mathbf{u}_p\right)\Delta t^2$ (everything at time t_n).

coupling) [2], the hydrodynamic radius of the particle is determined by the width of the kernel, which in turns is proportional to the mesh size. The evaluation of the hydrodynamic radius is done by performing momentum conserving simulations of settling [2]. For a scheme based on the Stokes drag coupling $\mathbf{F}_p = \xi_{bare}(\mathbf{V}_p - \mathbf{u}_p)$, one gets $\frac{1}{R_H} = 1/a_0 + 1/gh + 2.84/L + O(L^3)$ where L is the periodic box size. The effective friction coefficient is thus the sum of the bare (input) friction ($a_0 = \xi_{bare}/(6\pi\eta)$) and that arising from the hydrodynamic field ($g\,h = \xi_{hydro}/(6\pi\eta)$). The DF approach instantaneously transfer the particle-fluid momentum; corresponding to $\xi_{bare} = \infty$. This is indeed what we observe when plotting R_H against L. We get $g = 0.89$ and the translational invariance of g is satisfied up to 1%.

The second set of simulations were carried out to analyze the drag force to a particle up to moderate Reynolds number $Re < 10$. Results for the drag force are compatible with those obtained by Padding and Louis [9] resolving solid 3D particles in a Stochastic Rotation Dynamics solver with slip boundary conditions at the particle surface. This result is consistent with the point-wise character of the model; whereby the fluid obviously slips at the (non-resolved) particle "surface".

Velocity profiles around the particle at low Reynolds number were found to perfectly match the theoretical results. In order to avoid finite size effects we solved the (Re= 0 limit) flow around a fixed sphere in a fluid with fixed velocity at distances R_L from the sphere center.

Another test was to reproduce the hydrodynamic force between to particles as a function of their relative distance. Under low Reynolds and distances somewhat larger than the particle diameter this force is described by the Oseen expression [2]; while as they come closer lubrication forces become important and eventually diverge at contact. The DF point particle scheme correctly reproduces Oseen forces and is able to trace the initial force increase due to lubrication, when the particle centers are about 1.5 diameters apart.

Quite interestingly, the instantaneous transfer of momentum between fluid and particle ensures that there is no extra dissipative channel in the particle motion (as occurs in Stokes coupling [2]). This means that the particle kinetic temperature thermalizes with the fluid and its velocity follows a Boltzmann distribution at the fluid temperature, without the need of extra noise terms in the particle motion. Under fluctuating hydrodynamics we have also checked that the time correlation of the particle velocity properly recovers the long-time algebraic tail ($(\nu t)^{3/2}$) [9]. Finally simulations for an array of particles under the presence of a stationary plane sound wave of frequency ω were performed to measure the acoustic force on the particles. Comparison was made with the theory developed by Gor'kov [3]. Three length scales govern this problem: the acoustic boundary layer $\delta = \sqrt{(}\nu/\omega)$ (with $\nu = \eta/\rho$) the wavelength $\lambda = c\,2\pi/\omega$ and the particle particle radius R. Simulations were performed for a small particle ($R_H/\lambda \simeq 0.044$) in the non-viscous regime ($\delta/R_h \simeq 0.27$). It is noted that Stokes coupling is only valid for $\delta/R_H >> 1$. The radius of the particle and the sound velocity across the particle c_p are the two only adjustable parameters. We found that simulations perfectly fit the theoretical prediction

if $R = 1.2R_H$ and $c_p = c_f$, where the solvent sound velocity c_f corresponds to water at $T = 300$K [8]. Density perturbations were kept at low Mach, according to the predicted limitation of the present formulation (see above).

In summary we have presented an extension of Direct Forcing in Eulerian-Lagrangian schemes which can solve inertial effects on the particle and it is naturally adapted to fluctuating hydrodynamics. The algorithm is quite easy to adapt from a Stokes coupling algorithm and can be used to solve low Mach number flows up to moderate particle Reynolds number $\mathrm{R}e < 10$. Future extension for arbitrary Ma and larger Re are underway. With these generalizations we expect this method to have an impact in the study of finite particle size effects in turbulent flows.

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